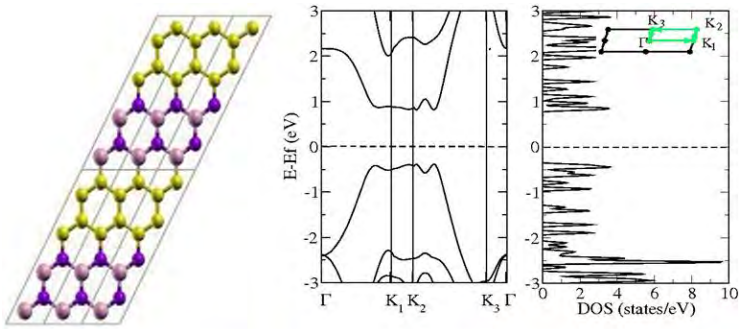
A report (dated September 20, 2011) on

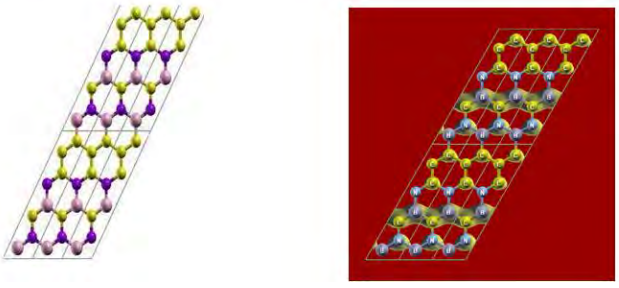
scientific research carried out under Grant: **FA2386-10-1-4150**

First-principles determination of thermal properties in nano-structured hexagonal solids with doping modifications for thermal energy harvesting

This is a continuation of the project no FA2386-10-1-4062 into the second year, and the present report has some overlap with the one submitted earlier.

1. **Defect Limited Thermal Conductivity of Graphene and related BCN systems:** Using the Quasi-continuum model of graphene developed in the first phase (reported in the last report), we estimate thermal conductivity of graphene with relaxation associated with scattering of phonons by topological Stone-Wales defects. This is being done using a Monte Carlo code (presently being developed) which simulates non-equilibrium state of the system by injecting heat (kinetic energy) at one plane and sinking it at another plane. These two planes have to be separated by more than the mean free path of phonons and thus, the system needs to be larger than 2 times the mean free path in direction of the thermal transport. Such an approach has been used by the author in the context of barium titanate, and we will implement it here for the quasi-continuum model of graphene.
   Work is in progress to estimate thermal conductivity using Kubo-Greenwood formula as well as the Fermi golden rule-based phenomenological approach. These three approaches will help in understanding thermal transport properties of graphene at a basic level.
   Similarly, the solution of BN and graphene (as being developed at the Wright-Patterson Lab by A Voevodin et al) has been extensively investigated, namely determination of their atomic structure and phonon properties:





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14. ABSTRACT
Using the Quasi-continuum model of grapheme developed in the first phase of the work, we estimated thermal conductivity of graphene with relaxation associated with scattering of phonons by topological Stone-Wales defects.

15. SUBJECT TERMS
thermal conductivity, graphene, thermal transport

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Figure1. Different atomic structures of BCN with domains of BN and graphene, and iso-surface of an electronic state localized at the boundary between such domains.

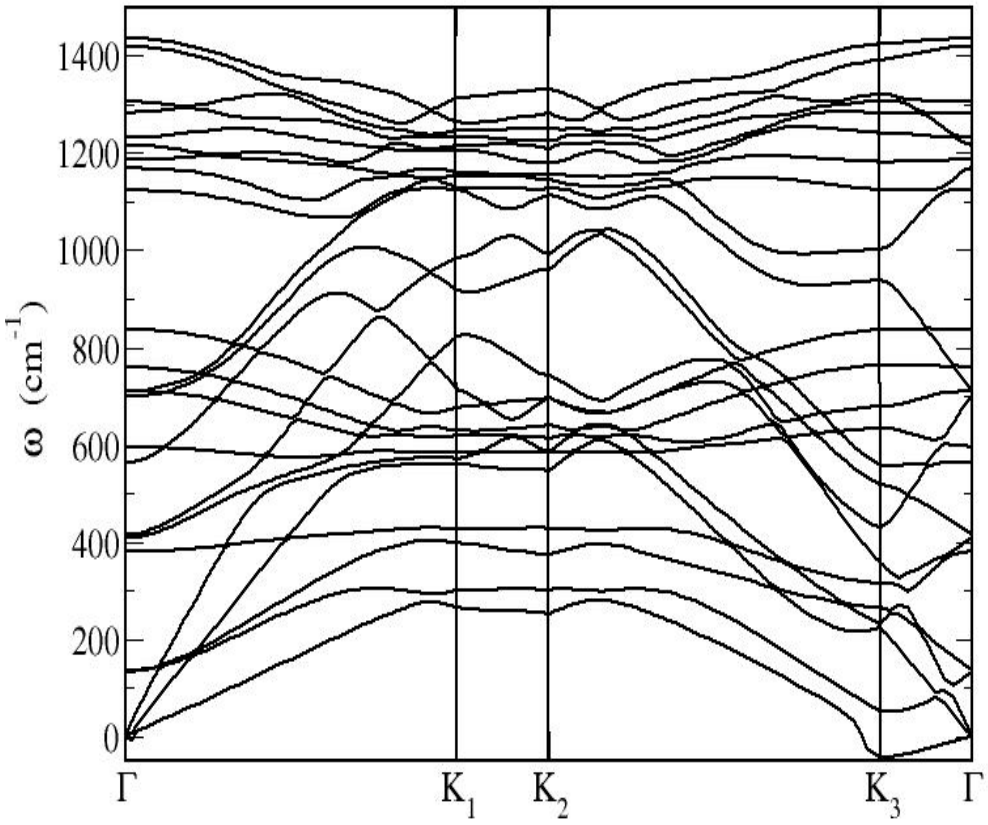

Figure 2. Phonon dispersion of BCN with domains of graphene and BN interfacing with each other along the zigzag direction.

Formulation developed above is being now used to determine thermal transport and related properties of BCN.

We also have carried out extensive analysis of Stone-Wales defects in BCN. Indeed, such defects can NOT form in BN due to its polar nature (energetically very expensive B-B and N-N bonds that would arise at such a defect). However, rather interesting situations can arise at the interface between BN and graphene (we are showing here only select configurations) :

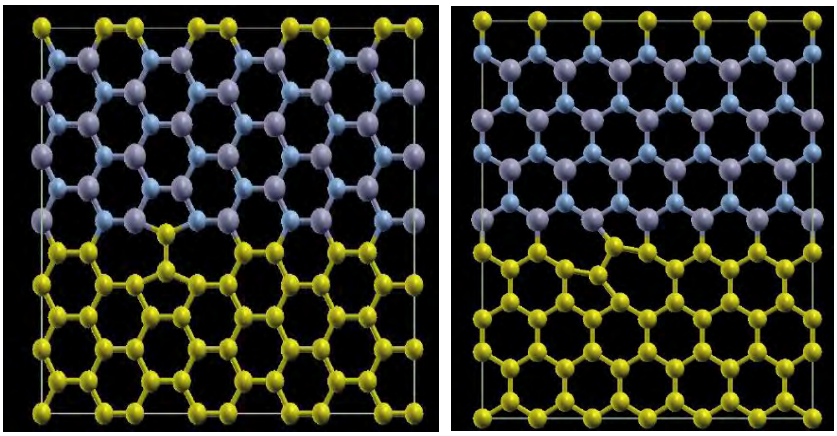

Figure 3. Novel Stone-Wales defects (which are lower in energy than the S-W defects in pristine graphene) at the BN-graphene interfaces in BCN. These cost energies of 4.26 and 4.06 eV for the defects in left and right panels respectively.

2. Metal-insulator transition in Solid Solution of BN and Graphene $(BN)_{1-x}C_x$ (BCN)

BCN has been one of the most interesting 2-dimensional hexagonal materials, particularly for its chemical and thermal properties. As BN is an insulating 2-D material and graphene is one with vanishing gap, their solid solution is expected to exhibit spectacular properties with spatial dependence. This has resulted in a very interesting paper based on recent experimental and theoretical works from groups of Ajayan and Louie et al [Ref. 1].

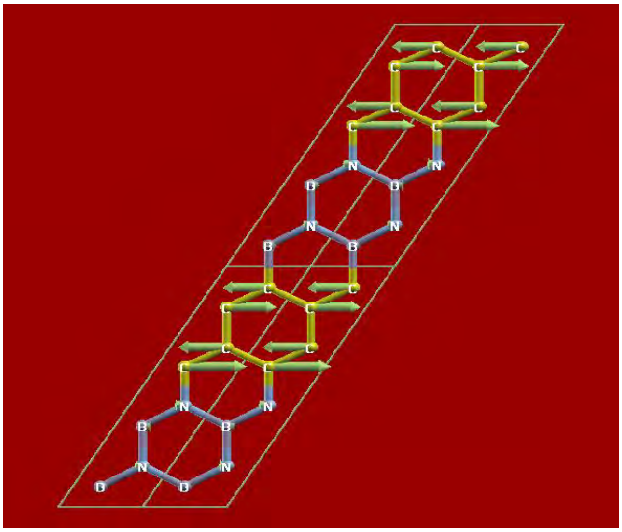

Figure. 4 Arrows show the force felt by different atoms due to applied electric field and it is evident that carbon atoms at the interface appear much more strongly ionic than B and N.

As shown in the first-phase, we find anomalous effective charges at the interfaces in BCN (see Figure 4). We have developed polaron model to explain high resistivity of BCN at elevated temperatures. Thus, we have a novel theory to explain the observations in Ref. 1, that is derived from first-principles.

3. Molybdenum sulphide:

We have demonstrated particularly strong electron phonon coupling for A and E phonons (see Figures 5, 6 below) in MoS_2. In collaboration with an experimental group (AK Sood et al), who made the first transistor based on MoS_2, we show how these modes and their Raman measurements can be used to characterize carrier doping in MoS_2 (manuscript under preparation). We are now investigating thermal

transport and storage properties of MoS_2.

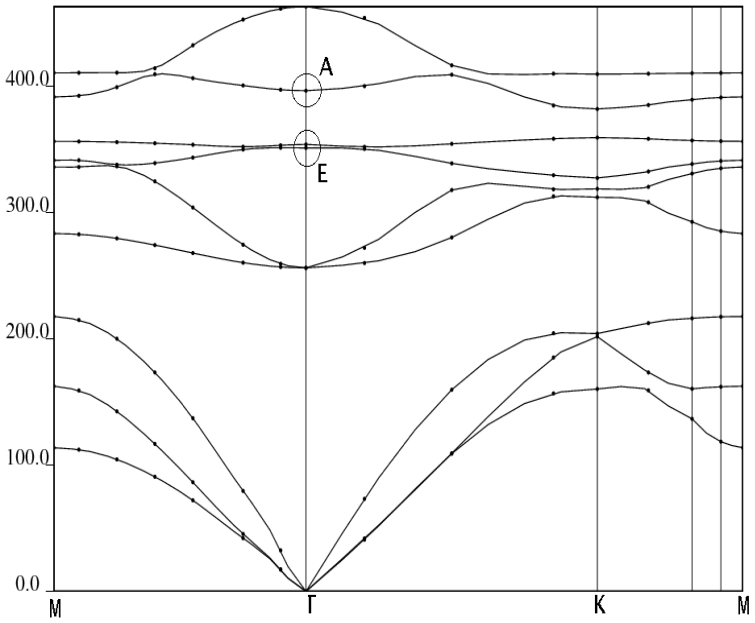

Figure 5. Phonon dispersion of MoS_2.

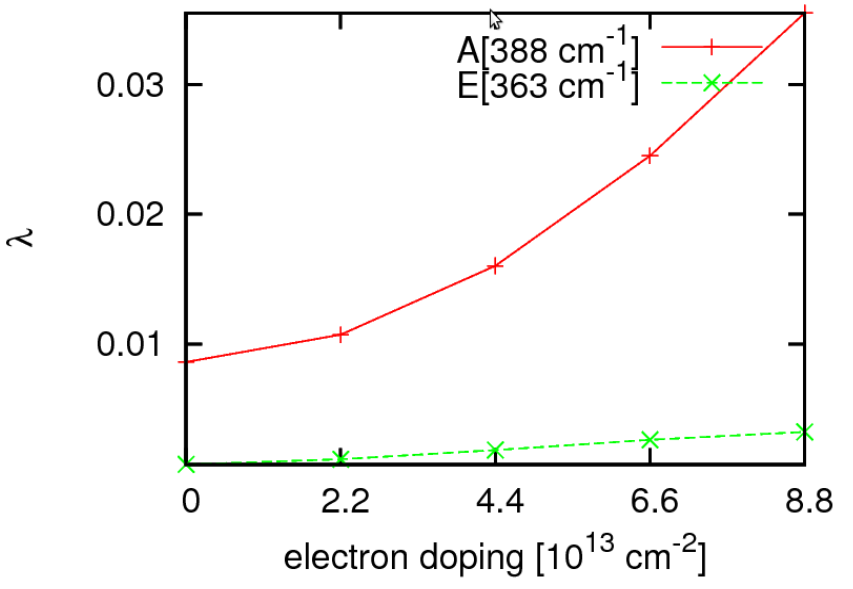

Figure 6. Electron-phonon coupling in MoS_2 as a function of carrier concentration.

References:

1. P M Ajayan et al, Nature Materials (2011).